Calculation of Vapor-Liquid Equilibria for a Ten Component System: Comparison of EOS, EOS-G^E and G^E-Henry's Law Models

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Vapor-liquid equilibrium data for a ten component system containing H2, CO, CO2, H2O, CH4, C2H6, C3H8, Methanol, Ethanol and n-Propanol have been used to evaluate the performance of several commonly used thermodynamic models for representing multi-component phase equilibrium data. The equation of state (EOS) used is the Soave-Redlich-Kwong (SRK) equation with modified mixing rules. The EOS-GE models used are the predictive Soave-Redlich-Kwong (PSRK) model by Fischer and Gmehling (1995), the MHV2 model by Dahl and Michelsen (1990) and the recently proposed model by Abovsky and Watanasiri (1998). The GE-Henry's law models used are the three popular activity coefficient models of Wilson, Uniquac and NRTL combined with the Henry coefficients derived from gas solubility data.

Application of the EOS-GE models to the mixture containing supercritical components such as those present in this work usually requires additional work to obtain binary parameters for the pairs involving these components. Some problems associated with handling supercritical components in the EOS-GE models are discussed and the results are shown for the bubble point pressure and vapor phase compositions at the conditions of pressure equal to 100 bar and temperature in the range of 313 – 333 K.